stn

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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JUL 28	CA/CAplus patent coverage enhanced
NEWS 3	JUL 28	EPFULL enhanced with additional legal status information from the epoline Register
NEWS 4	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 5	JUL 28	STN Viewer performance improved
NEWS 6	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS 7	AUG 13	CA/CAplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS 8	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS 9	AUG 15	CAplus currency for Korean patents enhanced
NEWS 10	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS 11	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS 12	SEP 25	CA/CAplus current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances
NEWS 13	SEP 26	WPIDS, WPINDEX, and WPIX coverage of Chinese and and Korean patents enhanced
NEWS 14	SEP 29	IFICLS enhanced with new super search field
NEWS 15	SEP 29	EMBASE and EMBAL enhanced with new search and display fields
NEWS 16	SEP 30	CAS patent coverage enhanced to include exemplified prophetic substances identified in new Japanese-language patents
NEWS 17	OCT 07	EPFULL enhanced with full implementation of EPC2000
NEWS 18	OCT 07	Multiple databases enhanced for more flexible patent number searching
NEWS 19	OCT 22	Current-awareness alert (SDI) setup and editing enhanced
NEWS 20	OCT 22	WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS 21	OCT 24	CHEMLIST enhanced with intermediate list of pre-registered REACH substances

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
specific topic.

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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 06:48:32 ON 27 OCT 2008

=> file casreact
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'CASREACT' ENTERED AT 06:48:45 ON 27 OCT 2008
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FILE CONTENT:1840 - 25 Oct 2008 VOL 149 ISS 18

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*************************************************************
*                                                           *
*     CASREACT now has more than 15.3 million reactions     *
*                                                           *
*************************************************************

CASREACT contains reactions from CAS and from: ZIC/VINITI database
(1974-1999) provided by InfoChem; INPI data prior to 1986;
Biotransformations database compiled under the direction of
Professor Dr. Klaus Kieslich; organic reactions, portions copyright
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This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\365.str
```

Updated Search

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L1      STRUCTURE UPLOADED

=>  s l1, crd ibib abs, fhit,
          2540 'L1'
             2 CRD
             0 IBIB
         16097 ABS
             3 FHIT
L2           0 L1, CRD IBIB ABS, FHIT,
                 ('L1'(W)CRD(W)IBIB(W)ABS(W)FHIT)

=> d l1, ibib abs crd, fhits
L1 HAS NO ANSWERS
'IBIB ABS CRD FHITS ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
ENTER STRUCTURE FORMAT (SIM), NOS:end

=> d l1, ibib abs crd, fhitsr
L1 HAS NO ANSWERS
'IBIB ABS CRD FHITSR ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
ENTER STRUCTURE FORMAT (SIM), NOS:end

=> s l1
SAMPLE SEARCH INITIATED 06:58:26 FILE 'CASREACT'
SCREENING COMPLETE -      179 REACTIONS TO VERIFY FROM       35 DOCUMENTS

100.0% DONE     179 VERIFIED       0 HIT RXNS                      0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:      2778 TO     4382
PROJECTED ANSWERS:               0 TO        0

L3            0 SEA SSS SAM L1 (     0 REACTIONS)

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 117.50 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 06:58:30 FILE 'CASREACT'
SCREENING COMPLETE -     5687 REACTIONS TO VERIFY FROM      617 DOCUMENTS

100.0% DONE    5687 VERIFIED      70 HIT RXNS                     23 DOCS
SEARCH TIME: 00.00.02

L4           23 SEA SSS FUL L1 (    70 REACTIONS)

=> d l4, ibib abs fhitstr, 1-23
'FHITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers



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CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number. SCAN must be entered on the same line as DISPLAY, e.g., D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with CA reference information (SO, PY). (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction Summary for all hit reactions and fields containing hit terms
OCC -------- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

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To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):end

=> d his

(FILE 'HOME' ENTERED AT 06:48:32 ON 27 OCT 2008)

FILE 'CASREACT' ENTERED AT 06:48:45 ON 27 OCT 2008
L1 STRUCTURE UPLOADED
L2 0 S L1, CRD IBIB ABS, FHIT,
L3 0 S L1
L4 23 S L1 FULL

=> d l4, ibib abs fhitstr, 1-5
'FHITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

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ABS -------- GI and AB
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SIBIB ------- IBIB, no citations

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those hit reactions whose steps are totally included
within another hit reaction which is displayed

To display a particular field or fields, enter the display field
codes. For a list of the display field codes, enter HELP DFIELDS
at an arrow prompt (=>). Examples of combinations include: D TI;
D BIB RX; D TI, AU, FCRD. The information is displayed in the same order
as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may
be used with the DISPLAY command to display the record for a specified
Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):ed
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The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data

Updated Search

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IPC -------- International Patent Classifications
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SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
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             hit reaction
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RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
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             contain a hit substance.  Also displays those
             multistep reactions that have a hit substance in both
             the first and last steps of the reaction, except for
             those hit reactions whose steps are totally included
             within another hit reaction which is displayed
```

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be used with the DISPLAY command to display the record for a specified
Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):end

=> d his

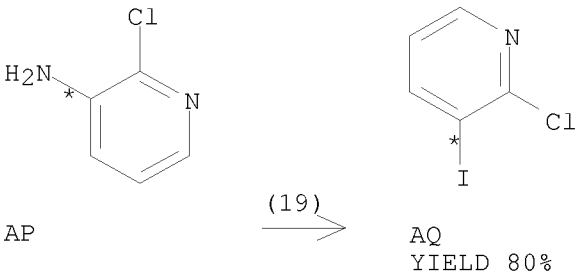
     (FILE 'HOME' ENTERED AT 06:48:32 ON 27 OCT 2008)

     FILE 'CASREACT' ENTERED AT 06:48:45 ON 27 OCT 2008
L1   STRUCTURE UPLOADED
L2   0 S L1, CRD IBIB ABS, FHIT,
L3   0 S L1
L4   23 S L1 FULL

=> d l4, fhit ibib abs, 1-23

L4   ANSWER 1 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(19) OF 22   AP ===> AQ



AP

AQ
YIELD 80%

RX(19)   RCT AP 6298-19-7

            STAGE(1)
               RGT C 104-15-4 TsOH
               SOL 75-05-8 MeCN
               CON room temperature -> 10 deg C

            STAGE(2)
               RGT D 7681-11-0 KI, E 7632-00-0 NaNO2
               SOL 7732-18-5 Water
               CON SUBSTAGE(1) 10 minutes, 10 - 15 deg C
                    SUBSTAGE(2) 10 deg C -> 20 deg C
                    SUBSTAGE(3) 50 minutes, 20 deg C

          PRO AQ 78607-36-0
ACCESSION NUMBER: 146:337774 CASREACT
TITLE: A new, one-step, effective protocol for the iodination
                         of aromatic and heterocyclic compounds via aprotic
                         diazotization of amines
AUTHOR(S):   Krasnokutskaya, Elena A.; Semenischeva, Nadya I.;
                         Filimonov, Victor D.; Knochel, Paul

Updated Search

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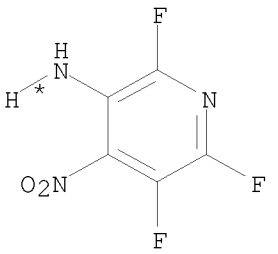
CORPORATE SOURCE: Department of Organic Chemistry, Tomsk Polytechnic University, Tomsk, 634050, Russia
SOURCE: Synthesis (2007), (1), 81-84
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have developed a convenient one-step preparation of aromatic and some heterocyclic iodides by the sequential diazotization-iodination of the aromatic amines with a Kl/NaNO2/p-TsOH system in acetonitrile at room temperature
This method has general character and allows aryl iodides with either donor or acceptor substituents in various positions to be obtained from the corresponding amines in 50-90% yield.

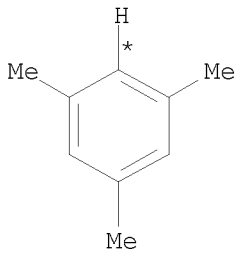
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(4) OF 39 ...J + N ===> O...

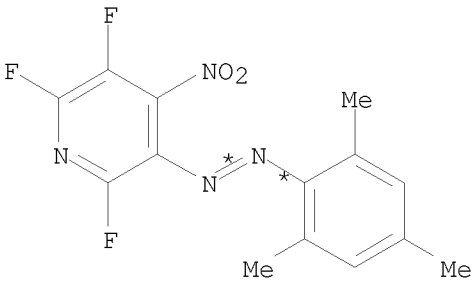


J



N

(4)



O
YIELD 84%

RX(4) RCT J 6226-46-6

Updated Search

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STAGE(1)
RGT P 7632-00-0 NaNO2, Q 7664-39-3 HF
SOL 7664-39-3 HF
CON SUBSTAGE(1) 5 minutes, room temperature
SUBSTAGE(2) 90 minutes, room temperature

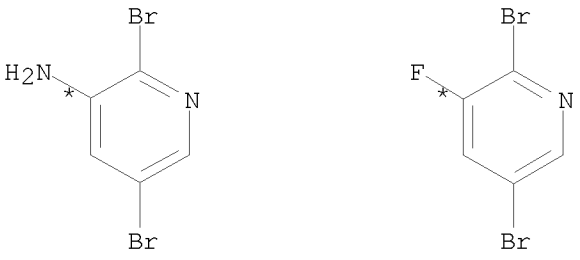
STAGE(2)
RCT N 108-67-8
CON room temperature

PRO O 322641-70-3

ACCESSION NUMBER: 145:188836 CASREACT
TITLE: Nucleophilic substitution in tetrafluoro-4-nitropyridine derivatives and the corresponding fluorinated diazepines: HPLC resolution of their isomers
AUTHOR(S): Sekhri, Lakhdar
CORPORATE SOURCE: Institut de Chimie Industriel, Universite de Ouargla, Ouargla, 30000, Algeria
SOURCE: Asian Journal of Chemistry (2005), 17(3), 1747-1766
CODEN: AJCHEW; ISSN: 0970-7077
PUBLISHER: Asian Journal of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Tetrafluoro-4-nitropyridine derivs. have been synthesized and separated successfully by HPLC. The resulting fluorinated amines and 4-amino-3-chlorotrifluoropyridine have also been diazotized and the resulting diazonium ions coupled to mesitylene giving the corresponding azo-compds. Treatment of these azo-compds. with sodium methoxide gave the corresponding methoxy(arylazo)perfluoropyridines. The thermolysis of the synthesized azo-compds. gave the corresponding diazepines in good yields. The structural diazepine-isomers were separated by HPLC.
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(102) OF 668 GF ===> GG...



GF → GG
YIELD 51%

Updated Search

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RX(102) RCT GF 90902-84-4

STAGE(1)
RGT FZ 7647-01-0 HCl, GH 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON SUBSTAGE(1) -5 deg C
SUBSTAGE(2) 30 minutes, -5 deg C

STAGE(2)
RGT GI 16940-81-1 H+ [PF6]-
SOL 7732-18-5 Water
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 1 hour, 0 deg C
SUBSTAGE(3) 90 deg C
SUBSTAGE(4) 90 deg C -> room temperature

STAGE(3)
RGT CI 144-55-8 NaHCO3
SOL 7732-18-5 Water
CON room temperature, basify

PRO GG 156772-60-0
NTE petroleum ether solvent used in 2nd stage

ACCESSION NUMBER: 143:422040 CASREACT
TITLE: Diarylalkyne compounds with MCH-receptor antagonistic activity, their preparation, pharmaceutical compositions, and use in therapy
PATENT ASSIGNEE(S): Boehringer Ingelheim International GmbH, Germany
SOURCE: U.S. Pat. Appl. Publ., 62 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050239826	A1	20051027	US 2005-104915	20050413
DE 102004017935	A1	20051103	DE 2004-102004017935 20040414	
CA 2559021	A1	20051103	CA 2005-2559021	20050408
WO 2005103031	A1	20051103	WO 2005-EP3683	20050408
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1740572	A1	20070110	EP 2005-716558	20050408
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				

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JP 2007532593 T 20071115 JP 2007-507706 20050408
PRIORITY APPLN. INFO.: DE 2004-102004017935200404 14
US 2004-563677P 20040420
WO 2005-EP3683 20050408
OTHER SOURCE(S): MARPAT 143:422040
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

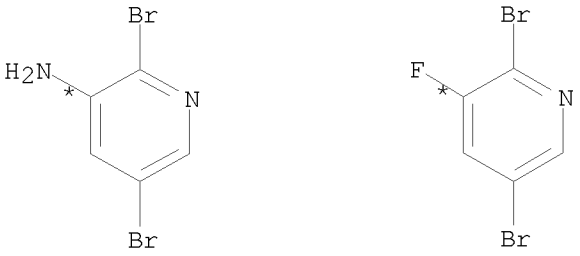
AB The invention relates to alkyne compds. of general formula I, which are antagonists of melanin-concentrating hormone (MCH) receptors. In compds. I, R1 is selected from C3-6 alkenyl, C3-6 alkynyl, (hydroxy-C3-7 cycloalkyl)-C1-3 alkyl, oxa-C4-7 cycloalkyl, and dihydroxy-C3-7 alkyl, each optionally substituted; R2 is independently selected from H, (un)substituted C1-8 alkyl, (un)substituted C3-7 cycloalkyl, (un)substituted Ph, (un)substituted pyridinyl, etc., or R1 and R2, together with the N atom to which they are bound, form an (un)substituted heterocycle; X is (un)substituted C1-4 alkylene; W and Z are each independently a bond or a C1-2 alkylene; Y and A are each independently (un)substituted Ph, (un)substituted pyridinyl, (un)substituted pyrimidinyl, (un)substituted pyrazinyl, etc.; B is (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl, (un)substituted C3-7 cycloalkyl, (un)substituted Ph, (un)substituted pyridinyl, etc.; including tautomers, enantiomers, salts, and mixts. thereof, with 6 specific compds. excluded. The invention also relates to the preparation of I, pharmaceutical compns. containing I and one or more physiol. acceptable excipients, inert carriers or diluents, as well as to the use of the compns. for the treatment of metabolic disorders and/or eating disorders, particularly obesity and diabetes. N-Alkylation of 3-methylpyridine with benzyl chloride followed by hydride reduction, asym. dihydroxylation, and debenzylation gave optically active piperidinediol II. 2-Bromoethanol underwent substitution with 4-iodo-2-methylphenol to give the corresponding ether, which was coupled with trimethylsilylacetylene and desilylated to give alkyne III. Coupling of III with 2,5-dibromopyridine, Suzuki coupling with 4-chlorophenylboronic acid, mesylation and substitution with piperidinediol II resulted in the formation of diarylalkyne IV. The compds. of the invention are MCH-receptor antagonists, with compound IV expressing an IC50 value of 10.9 nM.

L4 ANSWER 4 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(114) OF 747 KA ===> KB...

Updated Search

stn



RX(114) RCT KA 90902-84-4

STAGE(1)
RGT FQ 7647-01-0 HCl, DM 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON 30 minutes, -5 deg C

STAGE(2)
RGT KC 16940-81-1 H+ [PF6]-
SOL 7732-18-5 Water
CON 1 hour, 0 deg C

STAGE(3)
RGT DF 497-19-8 Na2CO3
SOL 7732-18-5 Water
CON SUBSTAGE(1) 90 deg C
SUBSTAGE(2) 90 deg C -> room temperature
SUBSTAGE(3) room temperature, basify

PRO KB 156772-60-0
NTE petroleum ether solvent used in stage 3 substage 1, regioselective

ACCESSION NUMBER: 143:405812 CASREACT
TITLE: Preparation of substituted pyridine alkynes with MCH antagonistic activity for the treatment of metabolic disorders
INVENTOR(S): Stenkamp, Dirk; Mueller, Stephan Georg; Lustenberger, Philipp; Lehmann-Lintz, Thorsten; Roth, Gerald Juergen; Rudolf, Klaus; Schindler, Marcus; Thomas, Leo; Lotz, Ralf
PATENT ASSIGNEE(S): Boehringer Ingelheim International GmbH, Germany
SOURCE: U.S. Pat. Appl. Publ., 67 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

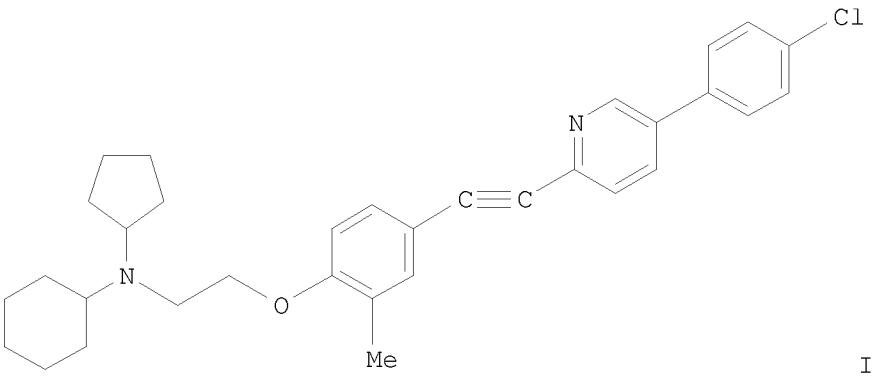
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050234101	A1	20051020	US 2005-104889	20050413

Updated Search

stn

DE 102004017934 A1 20051103 DE 2004-102004017934 20040414
CA 2559688 A1 20051103 CA 2005-2559688 20050408
WO 2005103002 A2 20051103 WO 2005-EP3685 20050408
WO 2005103002 A3 20060202
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
EP 1737823 A2 20070103 EP 2005-737015 20050408
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR
JP 2007532595 T 20071115 JP 2007-507708 20050408
PRIORITY APPLN. INFO.: DE 2004-102004017934 20040414
US 2004-563590P 20040420
WO 2005-EP3685 20050408

GI



II

AB Various substituted pyridinyl alkynes are prepared For instance, 2-[[4-[[5-(4-chlorophenyl)pyridin-2-yl]ethynyl]-2-methylphenyl]oxy]ethyl methanesulfonate (I) is prepared in 6 steps from 4-iodophenol, 2-bromoethanol, trimethylsilylacetylene, 2,5-dibromopyridine and 4-chlorophenylboronic acid. This intermediate is reacted with a variety of amines to produce example compds. I is converted to II by displacement with the corresponding amine. II exhibits an IC50 = 6.2 nM for MCH-1. Example compds. are useful for the treatment of metabolic disorders and/or eating disorders, particularly obesity and diabetes.

L4 ANSWER 5 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

Updated Search

stn

RX(1) OF 11 ...A ===> B

RX(1) RCT A 6298-19-7

STAGE(1)
RGT C 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature -> -8 deg C

STAGE(2)
RGT D 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON 30 minutes, -7 - -3 deg C

STAGE(3)
RGT C 7647-01-0 HCl
CAT 1317-38-0 CuO
SOL 109-69-3 BuCl, 7732-18-5 Water
CON 55 - 62 deg C

PRO B 2402-77-9

ACCESSION NUMBER: 143:155307 CASREACT
TITLE: Process for the manufacture of 2,3-dichloropyridine
INVENTOR(S): Shapiro, Rafael
PATENT ASSIGNEE(S): E.I. Dupont de Nemours and Company, USA
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005070888	A2	20050804	WO 2005-US2462	20050121

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,

Updated Search

stn

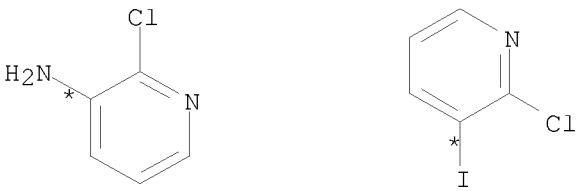
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2005206576	A1	20050804	AU 2005-206576	20050121
CA 2553850	A1	20050804	CA 2005-2553850	20050121
EP 1706381	A2	20061004	EP 2005-712075	20050121
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS, YU				
CN 1910152	A	20070207	CN 2005-80002691	20050121
BR 2005006502	A	20070227	BR 2005-6502	20050121
JP 2007523065	T	20070816	JP 2006-551437	20050121
US 20070161797	A1	20070712	US 2006-583635	20060620
IN 2006DN03640	A	20070824	IN 2006-DN3640	20060623
MX 2006PA08208	A	20060831	MX 2006-PA8208	20060719
PRIORITY APPLN. INFO.:			US 2004-539068P	20040123
			WO 2005-US2462	20050121

AB A method for preparing 2,3-dichloropyridine is disclosed in which 3-amino-2-chloropyridine is contacted with an alkali metal nitrite in the presence of aqueous hydrochloric acid to form a diazonium salt; and the diazonium salt is subsequently decomposed in the presence of copper catalyst wherein at least about 50% of the copper is the copper(II) oxidation state.

L4 ANSWER 6 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 115 J ===> B...



J

B
YIELD 92%

RX(2) RCT J 6298-19-7

STAGE(1)
RGT K 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature -> -5 deg C

STAGE(2)
RGT L 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON SUBSTAGE(1) <5 deg C
SUBSTAGE(2) 10 minutes, <5 deg C

STAGE(3)

Updated Search

stn

RGT M 7681-11-0 KI
SOL 7732-18-5 Water
CON SUBSTAGE(1) -5 deg C
SUBSTAGE(2) <10 deg C
SUBSTAGE(3) 0 deg C -> room temperature

STAGE(4)
RGT N 1310-73-2 NaOH
SOL 7732-18-5 Water, 141-78-6 AcOEt
CON room temperature, pH 11

PRO B 78607-36-0
NTE workup

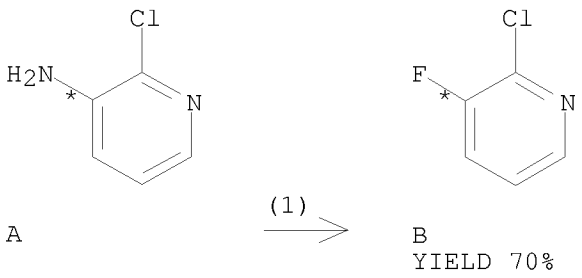
ACCESSION NUMBER: 141:410868 CASREACT
TITLE: Synthesis of Disubstituted Imidazo[4,5-b]pyridin-2-ones
AUTHOR(S): Kuethe, Jeffrey T.; Wong, Audrey; Davies, Ian W.
CORPORATE SOURCE: Department of Process Research, Merck & Co., Inc., Rahway, NJ, 07065, USA
SOURCE: Journal of Organic Chemistry (2004), 69(22), 7752-7754
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Regioselective palladium-catalyzed amination of 2-chloro-3-iodopyridine followed by a subsequent palladium-catalyzed amination leads to 2,3-diaminopyridines. Treatment with triphosgene affords highly functionalized unsym. imidazo[4,5-b]pyridin-2-ones in just three synthetic steps. A two-step synthesis of pseudosym. disubstituted imidazo[4,5-b]pyridin-2-ones, 1,4-disubstituted pyrido[2,3-b]pyrazinediones, and 1,3-disubstituted thiadiazolo[3,4-b]pyridin-2-ones is also described.

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(1) OF 23 A ===> B...



RX(1) RCT A 6298-19-7

STAGE(1)

Updated Search

stn

RGT C 16872-11-0 HBF4
SOL 7732-18-5 Water, 64-17-5 EtOH
CON 15 minutes, -5 deg C

STAGE(2)
RGT D 110-46-3 Isoamyl nitrite
CON SUBSTAGE(1) 5 minutes, <0 deg C
SUBSTAGE(2) 30 minutes, <0 deg C

STAGE(3)
SOL 142-82-5 Heptane
CON SUBSTAGE(1) 2 hours, <0 deg C -> reflux
SUBSTAGE(2) reflux -> 0 deg C

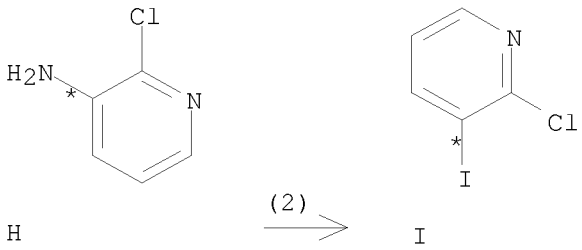
STAGE(4)
RGT E 1310-73-2 NaOH
SOL 7732-18-5 Water
CON 0 deg C -> room temperature

PRO B 17282-04-1
NTE thermal in stage 3

ACCESSION NUMBER: 140:423556 CASREACT
TITLE: Synthesis of 2-alkylamino-3-fluoropyridines using Buchwald conditions
AUTHOR(S): Munson, Peter M.; Thompson, Wayne J.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA, 19486, USA
SOURCE: Synthetic Communications (2004), 34(5), 759-766
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Synthesis of 2-alkylamino-3-fluoropyridines from 2-chloro-3-fluoropyridine using palladium-catalyzed coupling reaction under Buchwald conditions is described.
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 44 H ===> I...



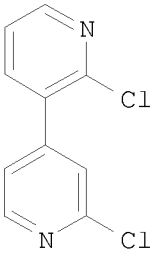
RX(2) RCT H 6298-19-7

Updated Search

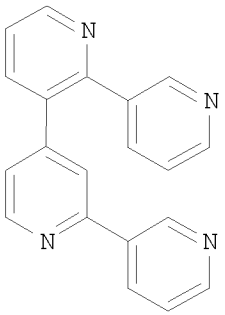
stn

RGT J 7647-01-0 HCl, K 7681-11-0 KI, L 7632-00-0 NaNO2
PRO I 78607-36-0
SOL 7732-18-5 Water

ACCESSION NUMBER: 140:93833 CASREACT
TITLE: An Efficient Two-Step Total Synthesis of the Quaterpyridine Nemertelline
AUTHOR(S): Bouillon, Alexandre; Voisin, Anne Sophie; Robic, Audrey; Lancelot, Jean-Charles; Collot, Valerie; Rault, Sylvain
CORPORATE SOURCE: UFR des Sciences Pharmaceutiques, Centre dEtudes et de Recherche sur le Medicament de Normandie, Caen, 14032, Fr.
SOURCE: Journal of Organic Chemistry (2003), 68(26), 10178-10180
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB Regioselective and univocal Suzuki cross-coupling reactions performed on halopyridinyl boronic acids provide a flexible and versatile route to a multigram scale synthesis of 2,2'-dichloro-3,4'-bipyridine (I), which allows couplings with excess pyridin-3-yl boronic acid to give a new and efficient two-step rapid synthesis of nemertelline (II), the quaterpyridine neurotoxin isolated from a Hoplonemertine sea worm.

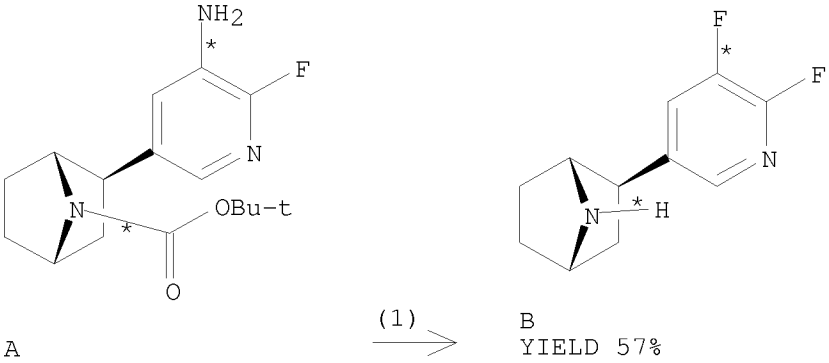
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(1) OF 95 ...A ===> B

Updated Search

stn



A

B
YIELD 57%

RX(1) RCT A 426462-05-7

STAGE(1)
RGT C 32001-55-1 4-MeOC6H4CPh2Cl
SOL 7732-18-5 Water

STAGE(2)
RGT D 7632-00-0 NaNO2

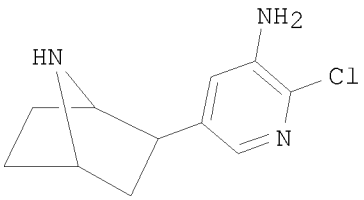
STAGE(3)
RGT E 1336-21-6 NH4OH
SOL 7732-18-5 Water

PRO B 426460-72-2

ACCESSION NUMBER: 137:353202 CASREACT
TITLE: Synthesis, Nicotinic Acetylcholine Receptor Binding, and Antinociceptive Properties of 2-exo-2-(2',3'-Disubstituted 5'-pyridinyl)-7-azabicyclo[2.2.1]heptanes: Epibatidine Analogues
AUTHOR(S): Carroll, F. Ivy; Lee, Jeffrey R.; Navarro, Hernan A.; Ma, Wei; Brieaddy, Lawrence E.; Abraham, Philip; Damaj, M. I.; Martin, Billy R.
CORPORATE SOURCE: Chemistry and Life Sciences, Research Triangle Institute, Research Triangle Park, NC, 27709, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(21), 4755-4761
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

Updated Search

stn



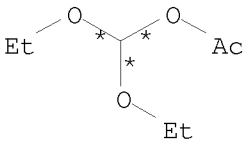
I

AB A number of 2',3'-disubstituted epibatidine analogs were synthesized and evaluated in vitro for potency at nicotinic acetylcholine receptors (nAChRs) and in vivo for antinociception activity in the tail-flick and hot-plate models of acute pain and for their ability to affect core body temperature Compds. that possessed electron-withdrawing groups (F, Cl, Br, and I) in both the 2'- and the 3'-positions showed affinities at the nAChR similar to epibatidine. However, in vivo efficacy did not correlate with affinity. 2-Exo-(3'-Amino-2'-chloro-5'-pyridinyl)-7-azabicyclo[2.2.1]heptane (I), an epibatidine analog possessing an electron-releasing amino group in the 3'-position, produced the highest affinity. Compound I was also the most selective epibatidine analog with a Ki of 0.001 nM at αβ nAChRs, which is 26 times greater than that of epibatidine, and a αβ/α7 Ki ratio of 14 000, twice that of epibatidine. In vivo testing revealed that this compound potently inhibited nicotine-induced antinociception with AD50 values below 1 μg/kg. Surprisingly, this same compound was also an agonist at higher doses (ED50 .apprx.20 μg/kg). Thus, the addition of the 3'-amino group to epibatidine confers potent antagonist activity to the compound with little effect on agonist activity. 2,3-Disubstituted epibatidine analogs possessing a 2'-amino group combined with a 3'-bromo or 3'-iodo group showed in vitro and in vivo nAChR properties similar to nicotine.

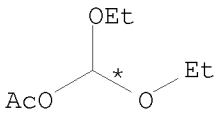
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

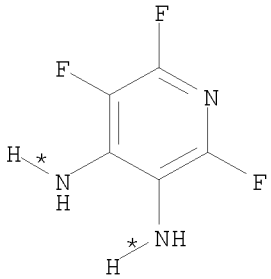
RX(26) OF 450 ...3 AR + 2 AM ===> AS + AT...



2 AR



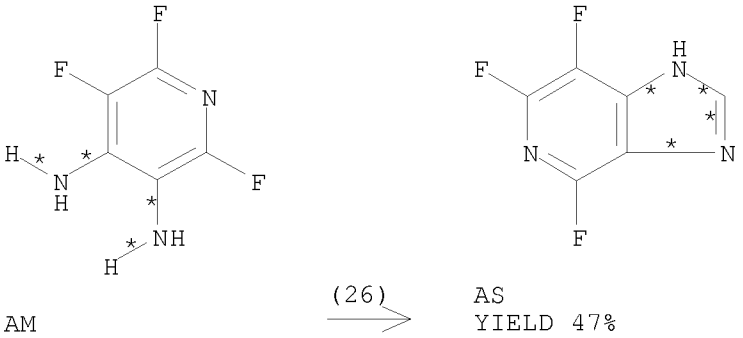
AR



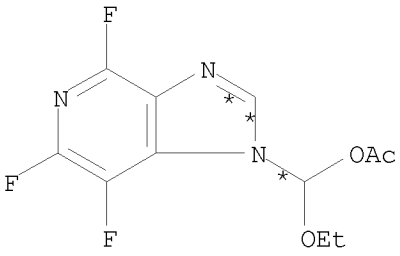
AM

Updated Search

stn



AM (26) AS YIELD 47%



AT
YIELD 28%

RX(26) RCT AR 14036-06-7, AM 6256-96-8
PRO AS 405230-95-7, AT 405231-20-1
ACCESSION NUMBER: 136:263363 CASREACT
TITLE: Synthesis of halogen-substituted 3-deazaadenosine and 3-deazaguanosine analogues as potential antitumor/antiviral agents
AUTHOR(S): Liu, Mao-Chin; Luo, Mei-Zhen; Mozdziesz, Diane E.; Lin, Tai-Shun; Dutschman, Ginger E.; Gullen, Elizabeth A.; Cheng, Yung-Chi; Sartorelli, Alan C.
CORPORATE SOURCE: Department of Pharmacology and Developmental Therapeutics Progam, Cancer Center, Yale University School of Medicine, New Haven, CT, 06520-8066, USA
SOURCE: Nucleosides, Nucleotides & Nucleic Acids (2001), 20(12), 1975-2000
CODEN: NNNAFY; ISSN: 1525-7770
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Various 2-halogen-substituted analogs, 3-halogen-substituted analogs, and 2',3'-dihalogen-substituted analogs of 3-deazaadenosine and 3-halogen-substituted analogs of 3-deazaguanosine have been synthesized as potential anticancer and/or antiviral agents. Among these compds., 3-deaza-3-bromoguanosine showed significant cytotoxicity against L1210, P388, CCRF-CEM and B16F10 cell lines in vitro, producing IC50 values of 3, 7, 9 and 7 μM, resp. Several 3-deazaadenosine analogs showed moderate

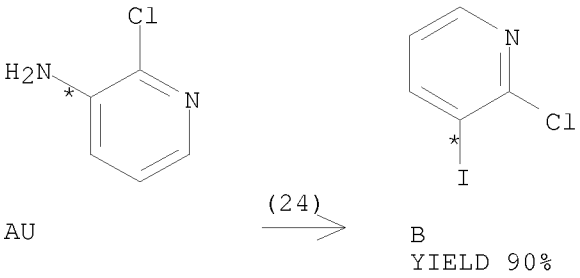
Updated Search

stn

to weak activity against hepatitis B virus.
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(24) OF 51 AU ===> B...



AU

B
YIELD 90%

RX(24) RCT AU 6298-19-7

STAGE(1)
RGT L 7647-01-0 HCl, AV 7632-00-0 NaNO2
SOL 7732-18-5 Water

STAGE(2)
RGT AW 7681-11-0 KI
SOL 7732-18-5 Water

PRO B 78607-36-0
ACCESSION NUMBER: 136:216632 CASREACT
TITLE: Coupling Reaction of Zirconacyclopentadienes with Dihalonaphthalenes and Dihalopyridines: A New Procedure for the Preparation of Substituted Anthracenes, Quinolines, and Isoquinolines
AUTHOR(S): Takahashi, Tamotsu; Li, Yanzhong; Stepnicka, Petr; Kitamura, Masanori; Liu, Yanjun; Nakajima, Kiyohiko; Kotora, Martin
CORPORATE SOURCE: Catalysis Research Center and Graduate School of Pharmaceutical Sciences, Hokkaido University, Japan
SOURCE: Journal of the American Chemical Society (2002), 124(4), 576-582
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Reactions of tetraiodobenzene with zirconacyclopentadienes, which were conveniently prepared from two alkynes (or diynes) and zirconocene complexes, afforded 1,2,3,4-tetrasubstituted diiodonaphthalene derivs. in good isolated yields. These 1,2,3,4-tetrasubstituted diiodonaphthalene derivs. could be converted to 1,2,3,4,5,6,7,8-octasubstituted anthracene derivs. by reaction with a second zirconacyclopentadiene. When the two zirconacyclopentadienes were different, unsym. anthracenes such as

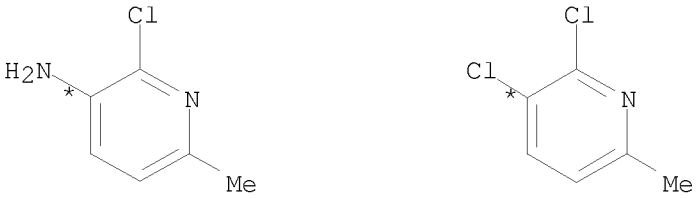
Updated Search

1,2,3,4-tetraethyl-5,6,7,8-tetraphenylanthracene (68% isolated yield) were obtained. On the other hand, treatment of a 2,3-dihalopyridine such as 2-bromo-3-iodopyridine with zirconacyclopentadienes gave 5,6,7,8-tetrasubstituted quinoline derivs. in good to high yields. 3,4-Dihalopyridines such as 4-chloro-3-iodopyridine reacted with zirconacyclopentadienes to afford 5,6,7,8-tetrasubstituted isoquinoline derivs. in good to high yields.

REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(5) OF 30 ...F ===> L...



F L
YIELD 76%

RX(5) RCT F 39745-40-9
RGT J 7632-00-0 NaNO2, K 7647-01-0 HCl
PRO L 54957-86-7
NTE 5-10.deg., CHLORIDES

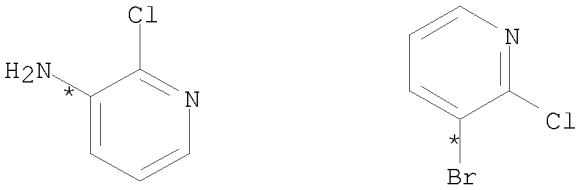
ACCESSION NUMBER: 126:47080 CASREACT
TITLE: Synthesis of dihalopicoline N-oxides and their 4-nitro derivatives
AUTHOR(S): Ciurla, H.; Puszko, A.
CORPORATE SOURCE: Russia
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1996), (10), 1366-1371
CODEN: KGSSAQ; ISSN: 0132-6244
PUBLISHER: Latviiskii Institut Organicheskogo Sinteza
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Three aminohalo-substituted α- and β-picolines, six dihalo-substituted α- and β-picolines, six dihalo-substituted α- and β-picoline N-oxides, and six dihalo-4-nitropicoline N-oxides were synthesized in excellent yields. Some properties of the products were reported.

L4 ANSWER 13 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(1) OF 17 A ===> B

stn

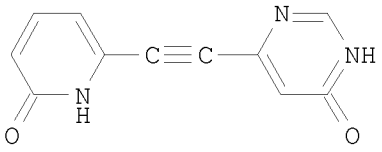


A

B
YIELD 91%

RX(1) RCT A 6298-19-7
RGT C 7632-00-0 NaNO2, D 7787-70-4 CuBr, E 10035-10-6 HBr
PRO B 52200-48-3
SOL 108-88-3 PhMe

ACCESSION NUMBER: 122:186872 CASREACT
TITLE: Use of Hydrogen Bonds to Control Molecular Aggregation. Behavior of Dipyridones and Pyridone-Pyrimidones Designed To Form Cyclic Triplexes
AUTHOR(S): Boucher, Eric; Simard, Michel; Wuest, James D.
CORPORATE SOURCE: Departement de Chimie, Universite de Montreal, Montreal, QC, H3C 3J7, Can.
SOURCE: Journal of Organic Chemistry (1995), 60(5), 1408-12
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

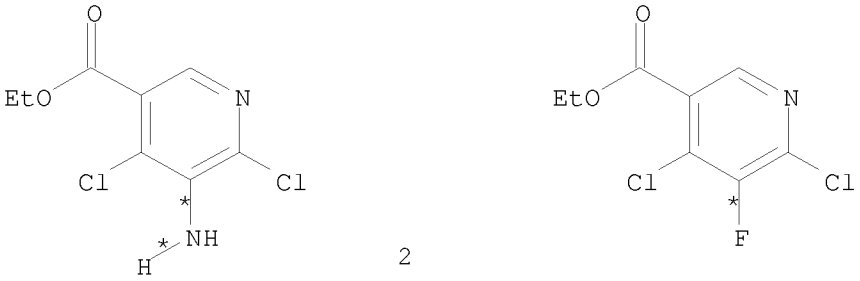
AB The tendency of 2-pyridones and related heterocycles to form cyclic hydrogen-bonded dimers allows them to be used as sticky sites that induce mols. in which they are incorporated to associate in particular ways. I, which is constructed from pyridone and pyrimidone subunits linked to a rigid linear acetylenic spacer, incorporates an array of hydrogen-bonding sites designed to favor the formation of a cyclic triplex. I was prepared and the structure of its DMSO solvate was determined by X-ray crystallog. Aggregation does not produce a cyclic triplex but rather gives chains in which adjacent mols. of I are linked by single hydrogen bonds.

L4 ANSWER 14 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(14) OF 66 COMPOSED OF RX(4), RX(5)
RX(14) J ===> R

Updated Search

stn

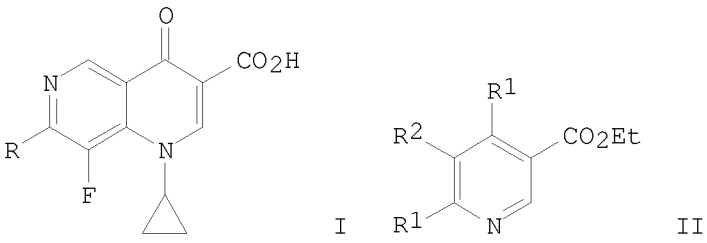


J R
YIELD 27%

RX(4) RCT J 154012-16-5
RGT O 16940-81-1 H+ [PF6]-, P 7632-00-0 NaNO2
PRO N 154012-09-6
SOL 7732-18-5 Water

RX(5) RCT N 154012-09-6
PRO R 154012-17-6
NTE thermal; key step

ACCESSION NUMBER: 120:244961 CASREACT
TITLE: The synthesis of a series of 7-amino-1-cyclopropyl-8-fluoro-1,4-dihydro-4-oxo-1,6-naphthyridine-3-carboxylic acids as potential antibacterial agents
AUTHOR(S): Sanchez, Joseph P.; Gogliotti, Rocco D.
CORPORATE SOURCE: Parke-Davis Pharm. Res. Div., Warner-Lambert Co., Ann Arbor, MI, 48105, USA
SOURCE: Journal of Heterocyclic Chemistry (1993), 30(4), 855-9
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I II

AB A series of title compds. I [R = 3-aminopyrrolidin-1-yl, 3-(ethylaminomethyl)pyrrolidin-1-yl, 4-aminopiperidin-1-yl, piperazin-1-yl] was prepared and evaluated for antibacterial activity (no data). I were prepared by the displacement of the chloro substituent from I (R = Cl) with the requisite nitrogen nucleophile. The naphthyridine acid was synthesized in ten steps from pyridinecarboxylate II (R1 = OH, R2 = NO2). The key step in the sequence was a Schiemann reaction of II (R1 =

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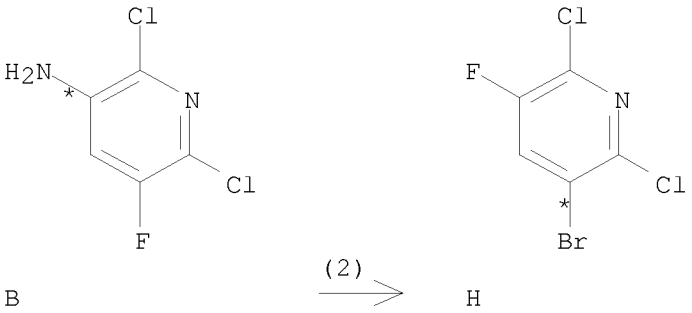
stn

Cl, R2 = N2+ PF6-) to give II (R1 = Cl, R2 = F).

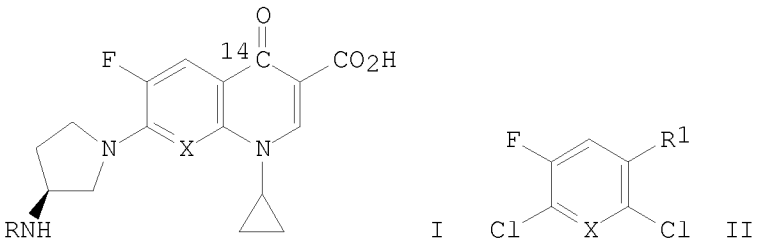
L4 ANSWER 15 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(2) OF 4 ...B ===> H



RX(2) RCT B 152840-65-8
RGT I 7787-70-4 CuBr, J 10035-10-6 HBr
PRO H 152840-66-9
NTE NANO

ACCESSION NUMBER: 120:107714 CASREACT
TITLE: A synthetic approach to carbon-14 labeled antibacterial naphthyridine- and quinolonecarboxylic acids
AUTHOR(S): Ekhato, I. Victor; Huang, Che C.
CORPORATE SOURCE: Parke-Davis Pharm. Res., Warner-Lambert Co., Ann Arbor, MI, 48105, USA
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1993), 33(9), 869-80
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Labeled versions of (S)-clinafloxacin (I; R = H, X = CCl) and two naphthyridinecarboxylic acid antibacterial compds. (I; R = H, H-Ala, X = N) were prepared Prepns. started from hitherto unknown bromo compds. II (R1 = Br), from which the corresponding 14C-labeled aromatic carboxylic acids II

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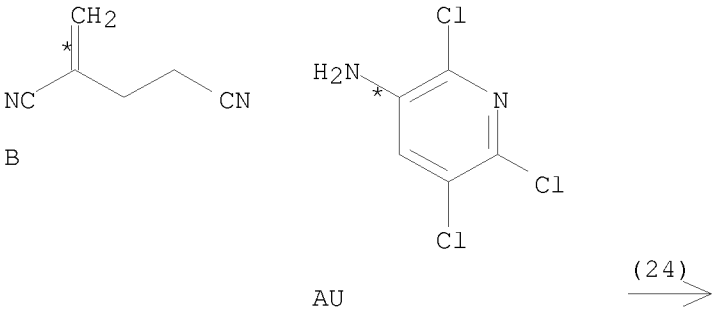
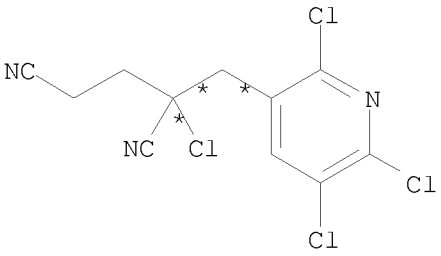
stn

(R = 14CO2H) were generated by metal-halogen exchange followed by carboxylation reaction. Details of these prepns. are given.

L4 ANSWER 16 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(24) OF 121 B + AU ===> AV





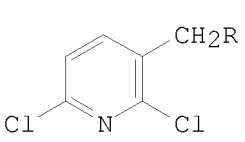
AV
YIELD 35%

RX(24) RCT B 1572-52-7, AU 55304-76-2
RGT D 7647-01-0 HCl, E 110-46-3 Isoamyl nitrite
PRO AV 112177-06-7
CAT 7758-89-6 CuCl
SOL 756-79-6 MeP(O)(OMe)2

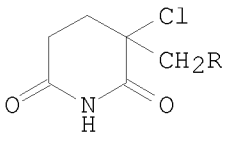
ACCESSION NUMBER: 108:55848 CASREACT
TITLE: The synthesis of halogenated pyridines substituted at the carbon atom C-3
AUTHOR(S): Sutter, Peter; Weis, Claus D.
CORPORATE SOURCE: Dyest. Chem. Dep., Ciba-Geigy, Ltd., Basel, Switz.
SOURCE: Journal of Heterocyclic Chemistry (1987), 24(4), 1093-102
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

Updated Search

stn



I

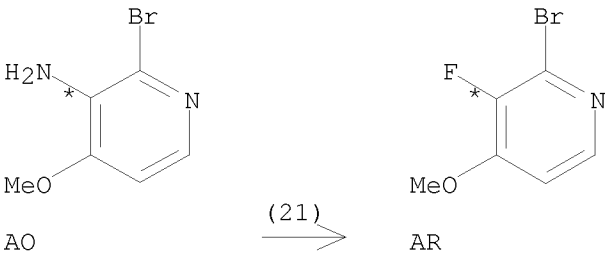


III

AB Seventeen 3-substituted pyridines I (R = Ph, 4-MeC6H4, 4-NO2C6H4, 2,5-Cl2C6H3, 3-pyridinyl, etc.) were prepared in 3 steps from the corresponding amines RNH2 (II). Arylation of H2C:C(CN)CH2CH2CN with II in the presence of CuCl, HCl, and isoamyl nitrite in di-Me methylphosphonate (preferred solvent) gave dicyanobutanes RCH2CCl(CN)CH2CH2CN which were cyclized with H2SO4-HOAc to give piperidinediones III. Aromatization with POCl3 in the presence of HMPA gave I.

L4 ANSWER 17 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(21) OF 90 ...AO ===> AR...



AO

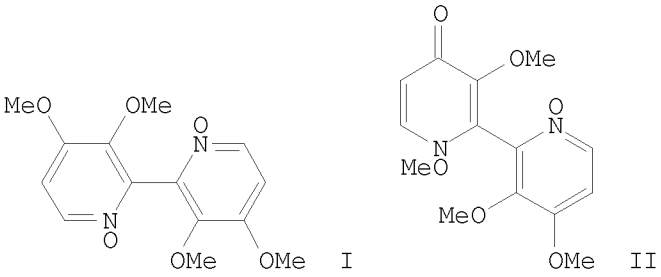
AR
YIELD 11%

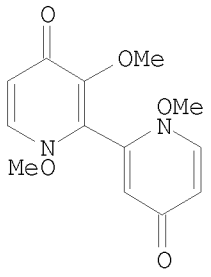
RX(21) RCT AO 109613-97-0
RGT AS 11113-50-1 Boric acid, AT 7664-39-3 HF, AU 110-46-3 Isoamyl nitrite
PRO AR 109613-98-1
SOL 7732-18-5 Water, 64-17-5 EtOH
NTE thermal diazonium salt decompn. in ligroin

ACCESSION NUMBER: 107:198450 CASREACT
TITLE: Syntheses of hydroxylated 2,2'-bipyridines. I. Orellanine, the poison of a toadstool
AUTHOR(S): Dehmlow, Eckehard V.; Schulz, Hans Joachim
CORPORATE SOURCE: Fak. Chem., Univ. Bielefeld, Bielefeld, D-4800, Fed. Rep. Ger.
SOURCE: Liebigs Annalen der Chemie (1987), (10), 857-61
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

Updated Search

stn

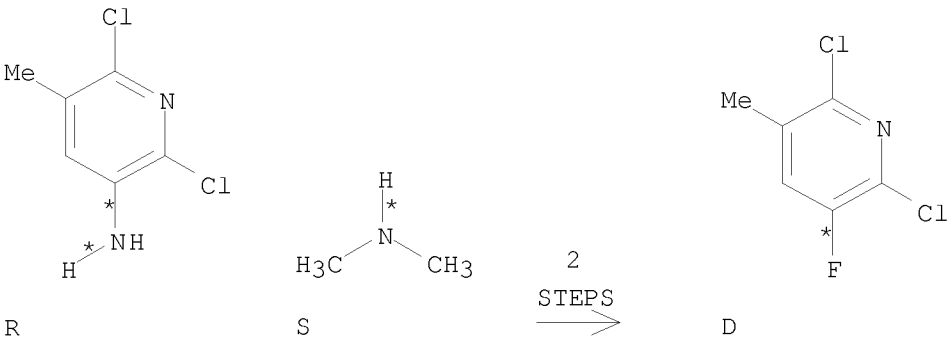




AB Orellanine (I) was prepared from 2-chloro-3-fluoropyridine or 3-amino-4-methoxypyridine via biaryl coupling of 2-chloro-3,4-dimethoxypyridine or 2-bromo-3-fluoro-4-methoxypyridine, resp. Reaction of I with CH2N2 gave bipyridines II and III. Results of UV irradiation of I are also given.

L4 ANSWER 18 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(35) OF 76 COMPOSED OF RX(9), RX(10)
RX(35) R + S ===> D



RX(9) RCT R 58596-89-7, S 124-40-3
RGT U 7647-01-0 HCl, V 7632-00-0 NaNO2
PRO T 104866-47-9

RX(10) RCT T 104866-47-9
RGT W 7664-39-3 HF

Updated Search

stn

PRO D 104866-49-1

ACCESSION NUMBER: 105:191059 CASREACT
TITLE: 1-Cyclopropyl-1,4-dihydro-4-oxo-1,8-naphthyridine-3-carboxylic acids
INVENTOR(S): Petersen, Uwe; Grohe, Klaus; Zeiler, Hans Joachim; Metzger, Karl Georg
PATENT ASSIGNEE(S): Bayer A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 64 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3508816	A1	19860710	DE 1985-3508816	19850313
NO 8505134	A	19860711	NO 1985-5134	19851218
NO 163331	B	19900129		
NO 163331	C	19900509		
EP 187376	A2	19860716	EP 1985-116551	19851224
EP 187376	A3	19880504		
EP 187376	B1	19920513		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
AT 76076	T	19920515	AT 1985-116551	19851224
US 4840954	A	19890620	US 1985-815440	19851231
IL 77538	A	19920525	IL 1986-77538	19860107
FI 8600073	A	19860711	FI 1986-73	19860108
FI 86721	B	19920630		
FI 86721	C	19921012		
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DD 257428	A5	19880615	DD 1986-296483	19860108
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DK 168439	B1	19940328		
JP 61161284	A	19860721	JP 1986-1485	19860109
JP 06053741	B	19940720		
ZA 8600163	A	19860924	ZA 1986-163	19860109
HU 40126	A2	19861128	HU 1986-87	19860109
HU 193623	B	19871130		
AU 8652164	A	19870122	AU 1986-52164	19860109
AU 574550	B2	19880707		
ES 550767	A5	19880715	ES 1986-550767	19860109
PL 148191	B1	19890930	PL 1986-264565	19860109
PL 148759	B1	19891130	PL 1986-257419	19860109
HU 202840	B	19910429	HU 1987-1847	19860109
CN 86100126	A	19860709	CN 1986-100126	19860110
CN 1003239	B	19890208		
NO 8600199	A	19860711	NO 1986-199	19860121
AU 8773118	A	19870910	AU 1987-73118	19870515
AU 576449	B2	19880825		
AU 8818359	A	19880915	AU 1988-18359	19880624
FI 8902675	A	19890601	FI 1989-2675	19890601
CA 1320206	C2	19930713	CA 1990-615694	19900405

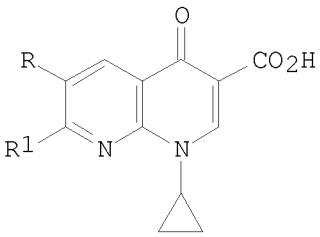
PRIORITY APPLN. INFO.: DE 1985-3500562 19850110

Updated Search

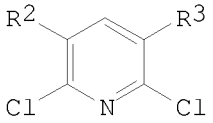
stn

DE 1985-3508816 19850313
EP 1985-116551 19851224
CA 1986-499241 19860108
FI 1986-73 19860108

OTHER SOURCE(S): MARPAT 105:191059
GI



I

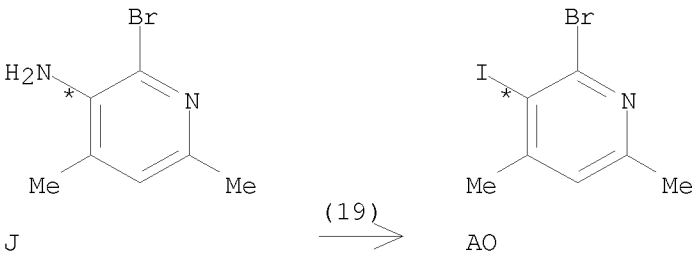


II

AB The title compds. [I; R = halo, NO2; R1 = (un)substituted 1-piperazinyl, 1-pyrrolidinyl] were prepared as bactericides and feed additives. Thus, 2,6-dichloro-5-methyl-3-pyridinamine (II, R2 = NH2, R3 = Me) was diazotized and coupled with Me2NH to give II (R2 = Me2NN:N, R3 = Me) which was fluorinated with HF to give II (R2 = F, R3 = Me). The latter was converted in 6 steps to II [R2 = F, R3 = EtO2CC(:CHOEt)CO] which was condensed with cyclopropylamine, followed by cyclization and hydrolysis of the ester group, to give I (R = F, R1 = Cl). The latter was heated with piperazine in Me2SO to give I (R = F, R1 = 1-piperazinyl) (III). III had a min. inhibitory concentration of ≤0.015 mcg/mL against Escherichia coli Neum. Tablets were prepared each containing III 583.0, microcyrst. cellulose 55.0, cornstarch 72.0, polyvinylpyrrolidine 30.0, dispersed silica 5.0, and Mg stearate 5.0 mg.

L4 ANSWER 19 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(19) OF 49 ...J ===> AO...



J

(19)

AO

RX(19) RCT J 104829-98-3

STAGE(1)
RGT AQ 7632-00-0 NaNO2, AR 7647-01-0 HCl

Updated Search

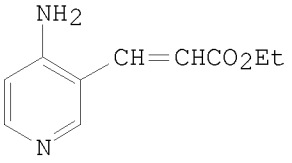
stn

SOL 7732-18-5 Water

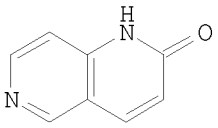
STAGE(2)
RGT AS 7681-11-0 KI
SOL 7732-18-5 Water

PRO AO 104830-09-3

ACCESSION NUMBER: 105:172323 CASREACT
TITLE: Condensed heteroaromatic ring systems. IV. Synthesis of naphthyridine derivatives by cyclization of aminopyridineacrylic esters
AUTHOR(S): Sakamoto, Takao; Kondo, Yoshinori; Yamanaka, Hiroshi
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(11), 4764-8
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

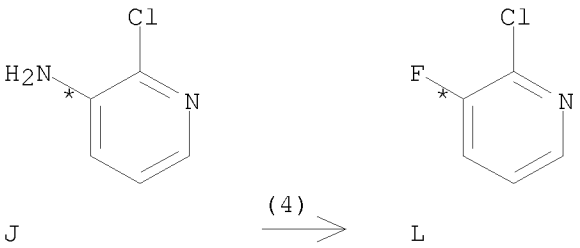


II

AB The reaction of aminohalopyridines with Et acrylate in the presence of palladium(II) acetate and triarylphosphine gave Et aminopyridineacrylates, e.g., I. The cyclization of the resulting acrylates under basic conditions gave naphthyridinones having a carbostyril-type moiety, e.g., II.

L4 ANSWER 20 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(4) OF 94 ...J ===> L...



J L

RX(4) RCT J 6298-19-7

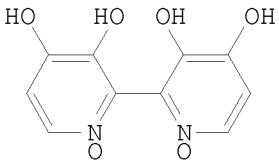
Updated Search

stn

STAGE(1)
RGT M 7782-77-6 HNO2

STAGE(2)
RGT N 16872-11-0 HBF4

PRO L 17282-04-1
ACCESSION NUMBER: 104:168236 CASREACT
TITLE: Synthesis of orellanine, the lethal poison of a toadstool
AUTHOR(S): Dehmlow, Eckehard V.; Schulz, Hans Joachim
CORPORATE SOURCE: Fak. Chem., Univ. Bielefeld, Bielefeld, D-4800/1, Fed. Rep. Ger.
SOURCE: Tetrahedron Letters (1985), 26(40), 4903-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

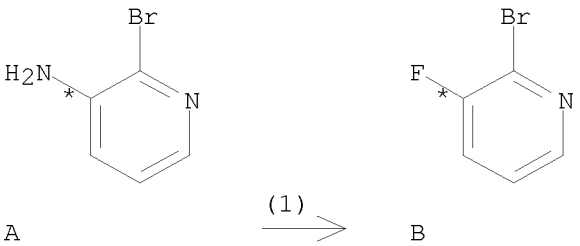


I

AB Orellanine, (I) was prepared in 10 steps from 3-aminopyridine, thus proving the identity of the natural product.

L4 ANSWER 21 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(1) OF 12 A ===> B...



A B

RX(1) RCT A 39856-58-1
PRO B 40273-45-8
CAT 16872-11-0 HBF4
ACCESSION NUMBER: 99:195034 CASREACT
TITLE: Review on the metalation of π-deficient heteroaromatic compounds. Regioselective

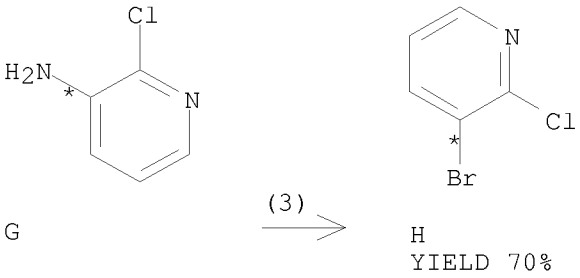
Updated Search

ortho-lithiation of 3-fluoropyridine: directing effects and application to synthesis of 2,3- or 3,4-disubstituted pyridines
AUTHOR(S): Marsais, Francis; Queguiner, Guy
CORPORATE SOURCE: Lab. Chim. Org. Heterocyclique, Inst. Natl. Super. Chim. Ind. Rouen, Mont Saint Aignan, 76130, Fr.
SOURCE: Tetrahedron (1983), 39(12), 2009-21
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB Lithiation of 3-fluoropyridine is chemoselective at low temps. using butyllithium-polyamine chelates or lithium diisopropylamide. Protophilic attack by these strong bases can be directed either at the 2- or 4-position depending on the lithiation conditions. Various reaction parameters are studied: solvent, temperature, reaction time, lithium-chelating agent metalating agent. The high regioselectivity of 3-fluoropyridine lithiation is theor. discussed, in particular in terms of kinetic or thermodn. control of the metalation. Chelation between butyllithium and 3-fluoropyridine is proposed, which completely modifies the heterocycle reactivity toward the lithiating agent. This is confirmed by theor. quantum calcns. performed on different models of 3-fluoropyridine using the CNDO/2. These results permit selection of 3-fluoropyridine metalation conditions which lead to 3-fluoro-2-lithiopyridine on the one hand and to 3-fluoro-4-lithiopyridine on the other hand. Each of the lithiated isomers is then reacted with a great variety of electrophiles to give the corresponding 2,3- or 3,4-disubstituted pyridines. Metalation of π-deficient heterocycles was also reviewed.

L4 ANSWER 22 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(3) OF 30 G ===> H...



G

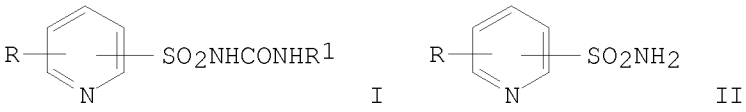
H
YIELD 70%

RX(3) RCT G 6298-19-7
RGT I 7782-77-6 HNO2, J 7787-70-4 CuBr
PRO H 52200-48-3
ACCESSION NUMBER: 88:152364 CASREACT
TITLE: Synthesis and pharmacological properties of certain alkylcarbamoylpyridinesulfonamides
AUTHOR(S): Delarge, J.
CORPORATE SOURCE: Inst. Pharm., Univ. Liege, Liege, Belg.
SOURCE: Acta Poloniae Pharmaceutica (1977), 34(3), 245-9

Updated Search

stn

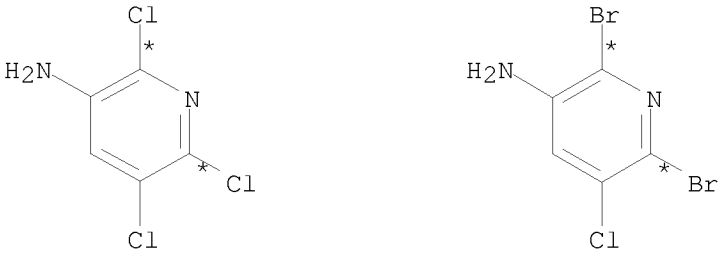
CODEN: APPHAX; ISSN: 0001-6837
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



AB Sixteen pyridine analogs I (R = 3-, 4-, 5-, 6-Me, 2-, 4-, 6-Cl, 3-Br, 4-Et2N, 4-Me2CHNH, 4-(3-ClC6H4)NH, 4-(3-CF3C6H4)NH; R1 = Et, Pr, Me2CH, Bu; SO2NHCONHR1 (in 2, 3, and 4 positions) of hypoglycemic sulfonamides were prepared from the appropriate II and R1NCO. II (R = 3-Br; SO2NH2 in 2 position) was prepared by converting 2-chloro-3-aminopyridine into 2-chloro-3-bromopyridine in a Sandmeyere reaction, then followed by reaction with KSH to give 3-bromopyridine-2-thiol, which was oxidized with Cl followed by amidation. I revealed no hypoglycemic activity; some of them were mild antiinflammatory agents. The 4-aryl-3-sulfonamide derivs. of the type I (R1 = Pr and Bu) were strong diuretics in expts. with animals as well as in clin. tests.

L4 ANSWER 23 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(15) OF 22 AD ===> AE



AD

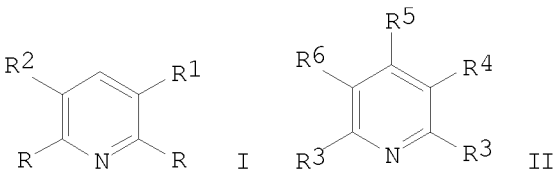
AE
YIELD 70%

RX(15) RCT AD 55304-76-2
RGT E 10035-10-6 HBr
PRO AE 55304-89-7
ACCESSION NUMBER: 84:121615 CASREACT
TITLE: Halogenated pyridines. V. Fluorinated and brominated pyridine compounds
AUTHOR(S): Mutterer, Francis; Weis, Claus D.
CORPORATE SOURCE: Div. Kunstst.-Addit. Farbst.-Chem., Ciba-Geigy A.-G., Basel, Switz.
SOURCE: Helvetica Chimica Acta (1976), 59(1), 229-35

Updated Search

stn

CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



AB Fluoropyridines I (R = F, R1 = Cl, Me, CF3, NO2, R2 = H, R1 = Cl, Me, R2 = Cl) were prepared by treating I (R = Cl, Br) with KF. I (R = Cl, R1 = CF3, R2 = H) was obtained by treating I (R = Cl, R1 =CCl3, R2 = H) with HF or SbF3. The bromopyridines II (R3 = Br; R4 = H, Cl, CH2R3, NO2, CHO, CO2H, CF3, NH2; R5 = H, R3; R6 = H, Cl, NO2) were obtained by brominating II (R3 = Cl) with HBr-HOAc.

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